MODELLING MIXING AND REACTION IN TURBULENT COMBUSTION

AFOSR Grant F-49620-97-1-0126

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Abstract

The most advanced probability density function (PDF) turbulent combustion models were developed and applied to make calculations of turbulent flames. The numerical accuracy of the calculations was carefully studied, and algorithmic improvements were developed. Various turbulence and combustion sub-models were developed and improved. The most significant achievement was the accurate calculation of the Sandia piloted jet nonpremixed flames, including quantitative predictions of local extinction, reignition, and minor species concentrations. Essential ingredients for these successful calculations were: the numerically-accurate particle-mesh method; the augmented reduced chemical mechanism; the in situ adaptive tabulation (ISAT) algorithm; and the Euclidean minimum spanning tree (EMST) mixing model.

INTRODUCTION

The design process for gas-turbine combustors and aerospace propulsion systems could be significantly improved if accurate and affordable CFD tools were available. While turbulent combustion models are used in the design process, the models currently employed are not sufficiently accurate. PDF methods promise the capability of greater accuracy, through their ability to treat the chemistry in sufficient detail, and to fully account for turbulence-chemistry interactions. The work performed in this research project has significantly contributed to the development and demonstration of PDF methods.

The research has focused on the following topics.

1/ PDF computations of the Sandia piloted jet nonpremixed flames.

2/ Development of algorithms and methodologies to improve the accuracy and efficiency of the particle/mesh methods used to solve the PDF equations.

3/ Development of turbulence-modelling aspects of PDF methods, including a model for turbulence frequency and applications to swirling flows.

4/ Development and testing of the Euclidean minimum spanning tree (EMST) mixing model (which overcomes deficiencies of earlier models).

5/ Development and demonstration of the PDF methodology as a subgrid scale model in large-eddy simulations.

The work on each topic is described in the following sections, and more completely in the publications given below.

PDF CALCULATIONS OF PILOTED JET FLAMES

The work in this area is fully described in the four papers Saxena & Pope (1998, 1999), Xu & Pope (2000) and Tang, Xu & Pope (2000). In each of these works PDF calculations are compared with the experimental data obtained at Sydney and Sandia. In each case, the PDF method is based on the joint PDF of velocity, frequency and composition, and uses the EMST mixing model and the ISAT algorithm to implement the chemistry.

In the computations of Saxena & Pope (1998, 1999) a C_1-skeletal mechanism for methane was used to calculate flame L measured by Masri, Dibble & Barlow (1996). This mechanism, because it contains no C_2 species, is unrealistic on the rich side. As a consequence the calculations of CO in particular are not very accurate.

To remedy this deficiency, Xu & Pope (2000) use the 16-species augmented reduced mechanism (ARM) developed by Sung, Law & Chen (1998); and Tang et al. (2000) use the 19-species ARM that includes NO_x chemistry. These calculations show excellent agreement compared to the experimental data of Barlow & Frank (1998).

A particular challenge for models applied to these flames is to predict the local extinction and subsequent reignition that occurs. Xu & Pope (2000) introduce a burning index to quantify these phenomena, and Fig. 1 compares the experimental and calculated values. It may be seen that, in general, the calculations are successful in predicting the dependence of the burning index on the fuel jet velocity and on downstream distance.

NUMERICAL METHODS FOR THE SOLUTION OF THE PDF EQUATIONS

Every numerical method involves numerical errors. In order to make accurate model calculations, and in order to assess the attributes of different physical sub-models, it is essential that the numerical errors are below tolerable limits.

In time-accurate CFD methods there are time-stepping errors and spatial truncation errors. For second-order accurate methods, these errors are of order Δt^2 and Δx^2, respectively, where Δt and Δx are the time step and the characteristic grid size. These same errors exist in particle/mesh methods; but in addition there are errors related to the average number of particles per cell, N. Comprehensive tests performed by Xu & Pope (1999) show that the time-stepping errors in the particle/mesh method are negligible, and that the remaining errors can be expressed as

$$\varepsilon = a\Delta x^2 + \frac{b}{N} + \frac{c\xi}{\sqrt{NM}}. \tag{1}$$

The last term is the *statistical error.* The coefficient c is the "standard error"; ξ is a standardized random variable ($\langle\xi\rangle = 0$, $\langle\xi^2\rangle = 1$); and M denotes the effective number of independent calculations. (Usually time averaging is used to reduce the statistical error: M is proportional to the number of time scales over which time averaging is performed.) The contribution with coefficient

b represents the *bias*. This is a deterministic error due to N being finite, and it is not reduced by time averaging. The term with coefficient a is the spatial *truncation error*.

The tests performed verify this behavior of the error and hence demonstrate the convergence of the scheme, i.e., ε tends to zero as Δx tends to zero and N tends to infinity. The rate of convergence is quantified by "measuring" the coefficients, a, b and c.

An extrapolation scheme (an extension of Richardson extrapolation) has been devised to eliminate the primary truncation error and bias. Two calculations are performed, with grid spacings Δx and $\sqrt{\alpha}\,\Delta x$, and numbers of particles N and αN, where α is a constant greater than one (e.g., $\alpha = 2$). Let Q_1 and Q_2 denote the value of some quantity obtained from the two calculations. It is apparent from Eq. (1) that the truncation error and bias in Q_2 is greater than that in Q_1 by a factor α. Consequently (to leading order), the quantity

$$Q_0 \equiv \frac{\alpha Q_1 - Q_2}{\alpha - 1}, \tag{2}$$

is free of these errors.

The efficacy of the extrapolation scheme is illustrated in Fig. 2. For the test case of a non-premixed piloted jet flame, the triangles show the numerical errors in calculations before extrapolation (i.e., in Q_1 and Q_2). The cases $A - E$ are for different choices of N, Δx and α. The circles and squares show (two variants of) the error in the extrapolated value (i.e., Q_0). Taking the turbulent kinetic energy (Fig. 2 d) cases $A - D$ as an example, before extrapolation the errors are in the range $7 - 22\%$: after extrapolation they are at most 3%.

While the particle/mesh code PDF2DV can be used to obtain accurate solutions to the modelled PDF transport equation, there are two motivations to develop alternative algorithms. The first is the fact that the bias in PDF2DV is unexpectedly large, and hence a large number of particles is required in order to make this numerical error acceptably small. An alternative algorithm, with smaller bias, would achieve the same accuracy at lower computational cost. The second motivation is to develop a PDF algorithm that can be combined with existing finite-volume codes, to facilitate technology transfer and the incorporation of the PDF methodology within existing LES codes.

The alternative numerical approach that has been developed is a completely consistent hybrid algorithm (Muradoglu et al. 1999, Jenny et al. 2000), consisting of a finite-volume (FV) code and particle code. The FV code solves the standard mean equations for the conservation of mass, momentum and energy, along with the mean equation of state. The particle method solves the modelled transport equation for the fluctuating velocity and thermochemical composition. The information exchanged between the codes is as follows: the mean velocity from the FV code is used in the particle code (to convect the particles); the various turbulent fluxes, the source of sensible energy and the mean molecular weight determined from the particles are used in the FV code. In contrast to previous hybrid algorithms (e.g., PDF2DS, Pope & Correa 1992), this method is completely consistent: there is no inconsistency between the fields represented in the two codes.

The results obtained (Jenny et al. 2000) show that these new hybrid methods offer efficiency gains of a factor of 100 or more.

TURBULENCE MODEL DEVELOPMENT

Accurate model calculations of turbulent combustion are possible only if the underlying turbulence model is accurate. Two advances have been made in the turbulence modelling aspects of PDF methods. The first is the development of a turbulent frequency model (Van Slooten, Jayesh & Pope 1998); the second is the development of a "wavevector model" which has the distinction of being exact in the rapid-distortion limit (Van Slooten & Pope 1997).

These new models were tested by Van Slooten & Pope (1999) for swirling jets (and other flows). Swirl is frequently used in combustion devices, to stabilize flames and to augment mixing. It is well known that simple turbulence models (e.g., the k-ε turbulence model) have difficulty in accurately representing swirling flows. To assess the accuracy of PDF methods for such flows, Van Slooten & Pope (1999) made calculations of the swirling jet studied experimentally by Takahashi et al. (1991). As an example of the results, Fig. 3 shows mean circumferential velocity profiles at different axial locations for the case of 30° swirl calculated using three variants of the PDF model. These and other results show that the wavevector model (solid line)—which is exact in the limit of rapid distortions—performs quite well, and is clearly superior to the less sophisticated Simplified Langevin Model.

THE EMST MIXING MODEL

The drive to make combustion chambers as compact as possible inevitably leads to operating conditions that can be close to extinction. A known deficiency of the popular IEM mixing model is that it incorrectly predicts extinction for non-premixed combustion at very high Damkohler numbers. The EMST mixing model is motivated by the need to overcome this deficiency. The model was developed under previous AFOSR funding and is described in Subramaniam & Pope (1998).

To test the efficacy of different models, the test case of "periodic reaction zones" has been studied (Subramaniam & Pope, 1999). In this problem the parameters are the Damkohler number Da, and the reaction zone thickness parameter $F \equiv \xi_R/\xi'$ (where ξ_R is the reaction zone thickness in mixture fraction space, and ξ' is the r.m.s. mixture fraction). For given F, there is a minimum value of Da for stable combustion, below which extinction occurs. This value of the critical Damkohler number according to different models is shown in Fig. 4. The smallest value of F ($F \approx 0.3$) corresponds to the flamelet regime. It may be seen that the EMST model and the conditional moment closure (CMC) yield comparable predictions. But IEM incorrectly predicts a value of Da larger by a factor of a thousand.

These results, together with those of Masri, et al. (1996), confirm the advantages of the EMST model.

LARGE-EDDY SIMULATION OF TURBULENT COMBUSTION

In collaboration with the group at SUNY Buffalo, we have implemented the PDF methodology as a subgrid scale combustion model in LES (Colucci et al. 1998, Jaberi et al. 1999, Giequel et al. 1998).

For turbulent combustion, LES has several attractions: large-scale unsteady motions and the effects of heat release are directly represented; and RANS turbulence modelling is avoided. It is important to appreciate, however, that, for the turbulence-chemistry interactions, LES faces the same formidable closure problem as statistical approaches. The challenge of simultaneously accounting for turbulent (subgrid scale) fluctuations and realistic finite-rate combustion chemistry is the same in LES as in statistical approaches—but in a much more costly computational setting.

As an illustration of this work, Fig. 5 shows DNS and LES calculations of a reactive mixing layer. With the neglect of subgrid-scale fluctuations, the calculated temperature is 40% too high; whereas the LES/PDF calculations are in good agreement with the DNS.

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2. P.J. Colucci, F.A. Jaberi, P. Givi and S.B. Pope (1998) "Filtered Density Function for Large Eddy Simulation of Turbulent Reacting Flows," Physics of Fluids, **10**, 499–515.

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6. P. Jenny, S.B. Pope, M. Muradoglu and D.A. Caughey (1999) "A new hybrid algorithm to solve the fully joint PDF equation for turbulent reactive flows," J. Comp. Phys. (submitted).

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11. V. Saxena and S.B. Pope (1998) "PDF Calculations of Major and Minor Species in a Turbulent Piloted Jet Flame," Twenty-seventh Symposium (Int'l) on Combustion, 1081–1086.

12. S. Subramaniam and S.B. Pope (1998) "A mixing model for turbulent reactive flows based on Euclidean minimum spanning trees," Combustion and Flame, **115**, 487–514.

13. S. Subramaniam and S.B. Pope (1999) "Comparison of mixing model performance for non-premixed turbulent reactive flow," Combustion and Flame, **117**, 732–754.

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21. J. Xu and S.B. Pope (1999) "Assessment of numerical accuracy of PDF/Monte Carlo Methods for Turbulent Reactive Flows," Journal of Computational Physics, **152**, 192–230.

PERSONNEL SUPPORTED

Prof. S.B. Pope, PI

Dr. V. Saxena, post-doc
Dr. P. Jenny, post-doc
S. Subramaniam
P.R. Van Slooten
J. Xu
S. Joseph

DEGREES GRANTED

S. Subramaniam, Ph.D.
P.R. Van Slooten, Ph.D.
J. Xu, Ph.D.

Shankar Subramaniam is now an Assistant Professor at Rutgers. Paul Van Slooten and Jun Xu are both working in the gas turbine industry, at UTRC and GE, respectively.

PUBLICATIONS

The following papers were written or published during the reporting period.

1. P.J. Colucci, F.A. Jaberi, P. Givi and S.B. Pope (1998) "Filtered Density Function for Large Eddy Simulation of Turbulent Reacting Flows," Physics of Fluids, **10**, 499–515.

2. F.A. Jaberi, P.J. Colucci, S. James, P. Givi and S.B. Pope (1999) "Filtered mass density function for large-eddy simulation of turbulent reacting flows," J. Fluid Mech. **401**, 85–121.

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10. S. Subramaniam and S.B. Pope (1998) "A mixing model for turbulent reactive flows based on Euclidean minimum spanning trees," Combustion and Flame, **115**, 487–514.

11. S. Subramaniam and S.B. Pope (1999) "Comparison of mixing model performance for non-premixed turbulent reactive flow," Combustion and Flame, **117**, 732–754.

12. Q. Tang, J. Xu and S.B. Pope (2000) "PDF calculations of local extinction and NO production in piloted-jet turbulent methane/air flames", Twenty-Eighth Symp. (Int'l) on Combust. (to be published).

13. P.R. Van Slooten and S.B. Pope (1999) "Application of PDF Modeling to Swirling and Non-swirling Turbulent Jets," Flow, Turbulence and Combustion, **62**, 295–333.

14. P.R. Van Slooten and S.B. Pope (1997) "PDF modeling of inhomogeneous turbulence with exact representation of rapid distortions," Physics of Fluids, **9**, 1085–1105.

15. P.R. Van Slooten, Jayesh and S.B. Pope (1998) "Advances in PDF modeling for inhomogeneous turbulent flows," Physics of Fluids, **10**, 246–265.

16. J. Xu and S.B. Pope (2000) "PDF calculations of turbulent nonpremixed flames with local extinction," Combust. Flame (to be published).

17. J. Xu and S.B. Pope (1999) "Assessment of numerical accuracy of PDF/Monte Carlo Methods for Turbulent Reactive Flows," Journal of Computational Physics, **152**, 192–230.

18. J. Xu and S.B. Pope (1998) "Turbulence modelling in joint PDF calculations of piloted-jet flames," 4th International Symposium on Engineering Turbulence Modelling and Measurements, Corsica, May 1999.

PRESENTATIONS

March 1997—AGTSR Combustion Workshop, Atlanta

April 1997—UTRC, invited talk, Hartford

May 1997—International Colloquium on Advanced Computation & Analysis of Combustion, invited talk, Moscow, Russia

May 1997—DOE 19th Combustion Research Conference, Chantilly, VA

June 1997—2nd International Workshop on Measurements and Computation of Turbulent Nonpremixed Flames, Heppenheim, Germany

June 1997—2nd International Symposium on Turbulence, Heat and Mass Transfer, invited talk, Delft, Netherlands

June 1997—ARO/AFOSR Contractors meeting in Chemical Propulsion, Ohio

August 1997—ICASE/LaRC/AFOSR Symposium on Modeling Complex Turbulent Flows, Hampton, VA

August 11-13, 1997—ICASE/LaRC/AFOSR Symposium on Modeling Complex Turbulent Flows, Invited Talk, Hampton, VA.

October 28-29, 1997—ATS Annual Meeting, FETC, Morgantown, WV.

November 23-25, 1997—American Physical Society, Division of Fluid Dynamics, 50th Annual Meeting, 3 Contributed Talks, San Francisco, CA.

December 8, 1997—University of Michigan, Aerospace Engineering, Invited Seminar, Detroit, MI.

December 9, 1997—General Motors Research, Invited Seminar, Warren, MI.

March 19, 1998—University of Michigan, Aerospace Engineering, Invited Seminar.

March 25–26, 1998—AGTSR Combustion Workshop, Berkeley, CA.

March 27, 1998—Rocketdyne, Talk on PDF methods for turbulent combustion, Canoga Park, CA.

June 29–July 1, 1998—AFOSR Contractors Meeting, Long Beach, CA.

July 30–31, 1998—Non-premixed Turbulent Flame Workshop, Boulder, Co.

August 5–27th, 1998 International Combustion Symposium, Boulder CO, Contributed talk.

November 23, 1998—51st Annual Meeting, APS/DFD, 2 contributed talks.

December 14, 1998—J.M. Burgers Center for Fluid Mechanics, Delft, Netherlands, Invited lecture.

December 15, 1998—Delft University of Technology, Invited lecture.

March 14–16, 1999—Joint Meeting of the Combustion Institute, 2 contributed talks.

April 18–20, 1999—AGTSR Combustion Workshop.

May 27, 1999—Delft University of Technology, Invited Lecture.

June 2–4, 1999—Reduced Mechanisms and Turbulent Combustion Workshop, Argonne National Laboratory, Invited Lecture.

June 9–11, 1999—DOE contractors' meeting, Lake Tahoe, CA.

June 14–16, 1999—AFOSR Contractors' meeting, Bar Harbour, Maine.

July 13–16, 1999—Reactive Turbulence Workshop, NCAR, Boulder CO, Invited Talk.

August 23, 24, 1999—Symposium on Fluid Mechanics and the Environment, Cornell, invited talk.

October 7, 1999—Pratt & Whitney Fellows Lecture, Hartford CT, invited lecture.

October 11, 12, 1999—Combustion Institute, Eastern States Meeting, invited plenary lecture.

November 8-10, 1999—Advanced Turbine Systems, Annual Meeting. Washington, DC, poster presentation.

November 21-23, 1999—American Physical Society, Division of Fluid Dynamics. 3 contributed talks.

January 19, 2000—Rutgers, invited seminar.

TECHNOLOGY TRANSITIONS AND TRANSFERS

The following technology transitions and transfers were reported in annual reports.

1997

Dr. M.S. Anand
Allison Engine Company
Indianapolis, IN
(317) 230–2828

1. EMST mixing model implemented in PDF code. For use in gas turbine combustor design code.
2. Wavevector model implemented in PDF code. For use in gas turbine combustor design code.

Dr. A.T. Norris
Ohio Aerospace Institute
22800 Cedar Point Rd.
Brook Park, OH 44142
(216) 962–3071

Dr. Norris has implemented the TGLDM method for simplified combustion chemistry into the National Combustor Code. The TGLDM (Trajectory Generated Low Dimensional Manifold) method was developed by the PI.

1998

Dr. M.S. Anand
Rolls Royce Allison
Indianapolis, IN
317-230-2828

PDF algorithm for non-orthogonal combustor code.

1999

Dr. Gal Berkooz
Beam Technologies
110 N. Cayuga St.
Ithaca, NY 14850
607-273-4367

PDF models and algorithms incorporated into the code PDF 3DS for use in aerospace applications.

Dr. M.S. Anand
Allison Engine Company
Indianapolis, IN
317-230-2828

PDF models and algorithm implemented in PDF module for the National Combustor Code.

OTHER INTERACTIONS

During the reporting period the PI has been a consultant to Rolls-Royce Allison, Boeing (Rocketdyne), General Motors and Beam Technologies. He has visited Rocketdyne, General Motors, UTRC, Pratt & Whitney and Beam Technologies. He has assisted in transferring the technologies developed at Cornell to industry by participating in SBIR's from AF and NASA.

PIADC INFORMATION

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Contract/Grant No.:	F49620-97-1-0126
Co-investigators:	Faculty – 0, Post-docs – 2, Graduate Students – 4
Publications—see above	
Honors/Awards:	Reporting period, appointed: Sibley College Professor, Cornell. J.B. Burgers Center Professor, University of Delft (visiting appointment)
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Fellow 1991, American Physical Society:	1991
Overseas Fellow, Churchill College, Cambridge:	1989
D. Sc. (Eng.), University of London:	1986
Associate Fellow, AIAA:	1984

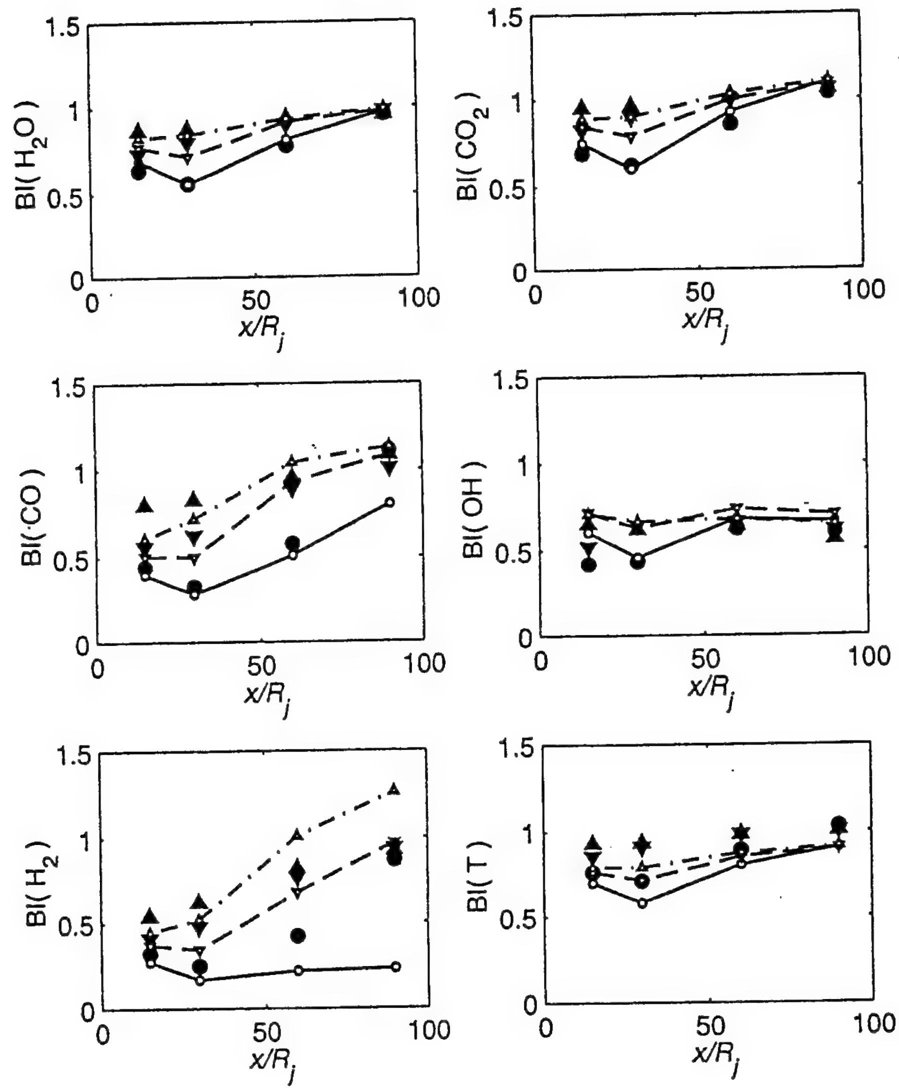

Figure 1: Burning indexes for the Barlow & Frank (1998) flames D, E and F (which have progressively higher jet velocities). Filled symbols, experiments; lines with empty symbols, PDF calculations. Circle and solid line, flame F; down-triangle and dashed line, flame E; up-triangle and dashed-dotted line, flame D. (From Xu & Pope 2000.)

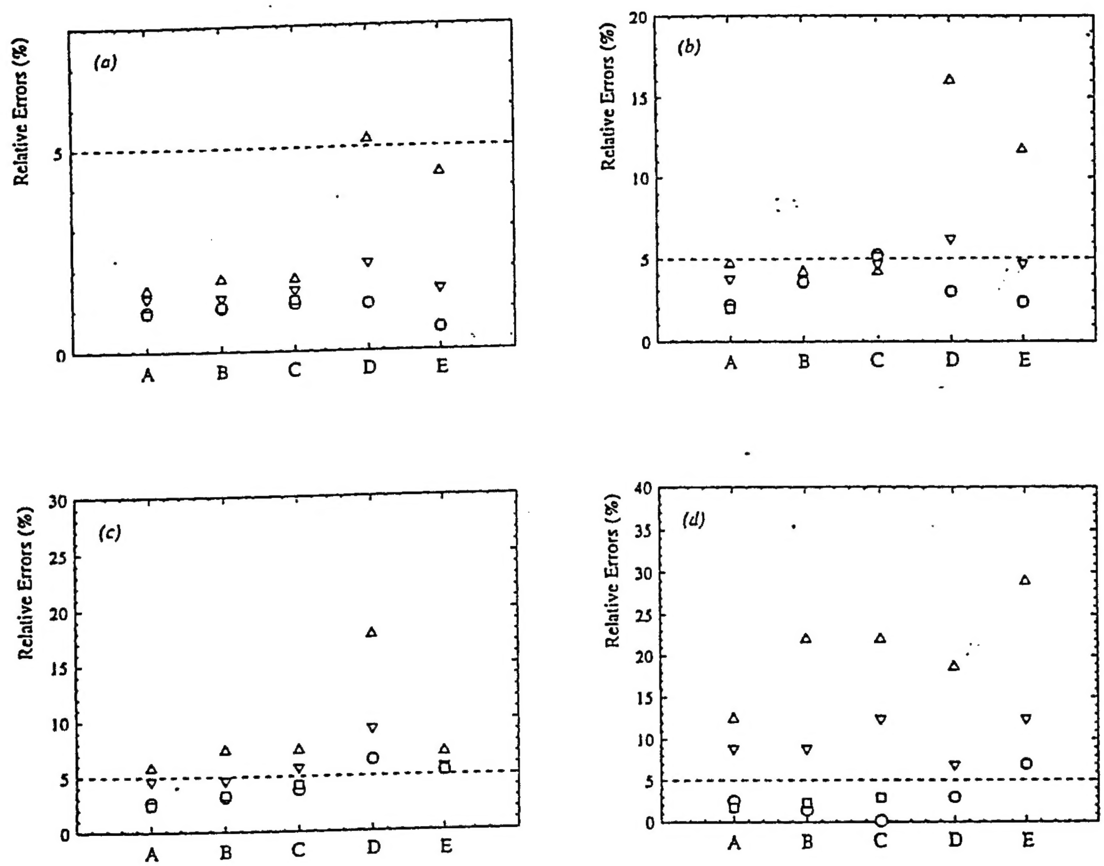

Figure 2: Relative errors in selected quantities in the non-premixed piloted jet flame test (a) mean velocity (b) mean mixture fraction (c) turbulence frequency (d) turbulent kinetic energy. Symbols: triangles, basic calculation; Squares and circles, extrapolated quantities. (From Xu & Pope 1999.)

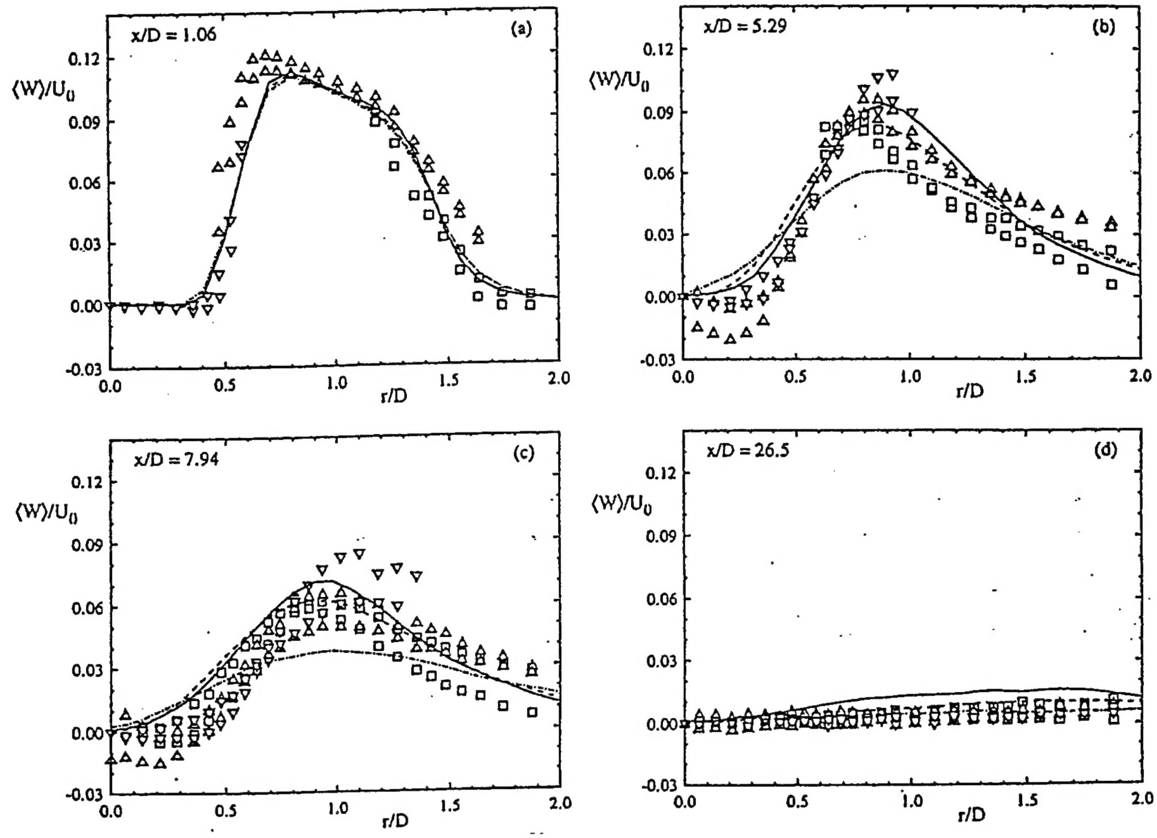

Figure 3: Mean circumferential velocity profiles at different axial distances in a 30° swirling jet. Symbols, experimental data of Takahashi et al. (1991); solid line, wavevector PDF model; dashed line, Lagrangian isotropization of production (LIPM) PDF model; dot-dashed line, Simplified Langevin PDF model. (From Van Slooten & Pope 1999.)

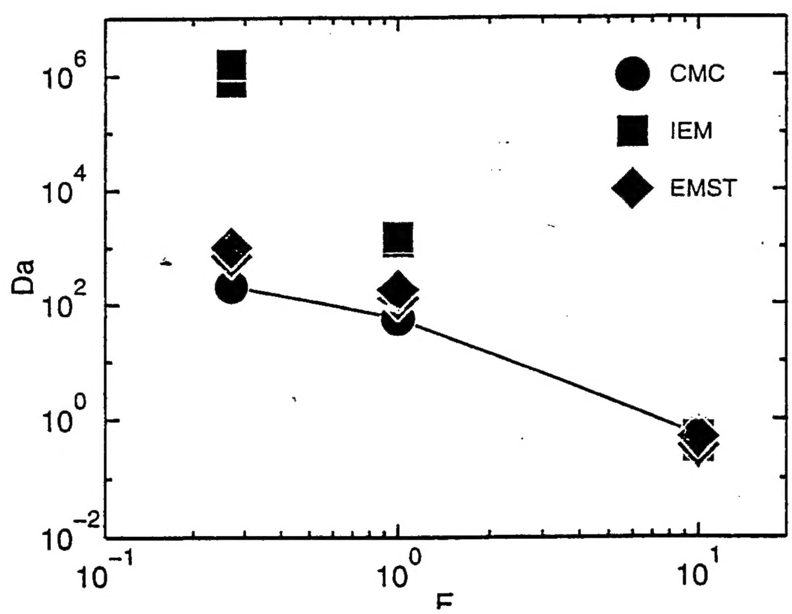

Figure 4: Predictions of critical Damkohler number for extinction against reaction zone thickness parameter $F = \varepsilon_R/\varepsilon'$ for different models (from Subramaniam & Pope, 1999).

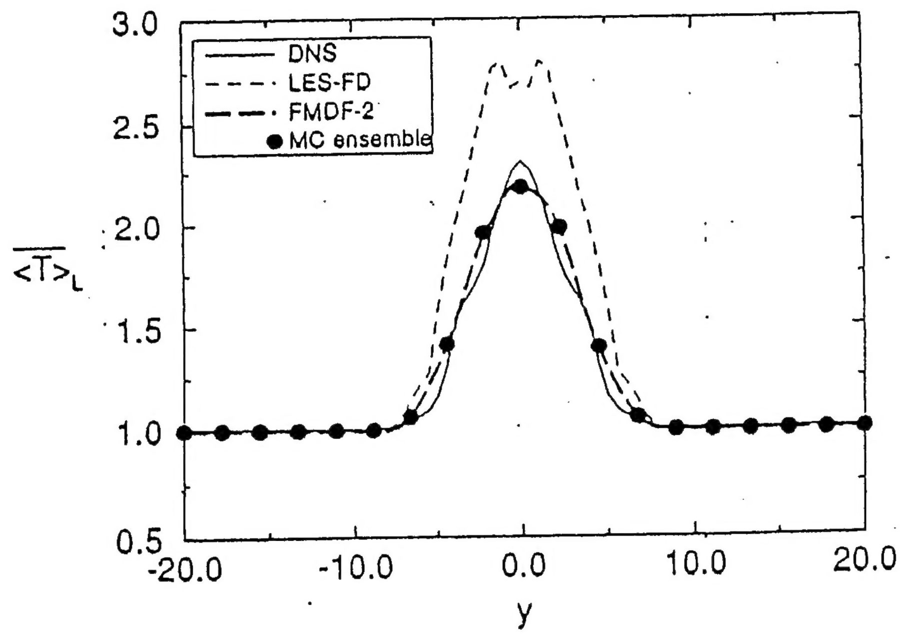

Figure 5: Mean normalized temperature profiles in a reactive turbulent mixing layer showing the agreement between DNS and LES using PDF methodology (denoted FMDF-2). In LES-FD subgrid-scale fluctuations are neglected. (From Jaberi et al. 1999.)

REPORT DOCUMENTATION PAGE

AFRL-SR-BL-TR-00-

0213

1. AGENCY USE ONLY (Leave blank)

2. REPORT DATE
00/5/8

3. REPORT TYPE AND DATES COVERED
Final Technical 97/2/15 - 00/2/14

4. TITLE AND SUBTITLE
(U) Modelling Mixing and Reaction in Turbulence Combustion

5. FUNDING NUMBERS
PE - 61102F
PR - 2308
SA - BX
G - F49620-97-1-0126

6. AUTHOR(S)
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR/NA
801 N. Randolph St. Room 732
Bolling AFB DC 20332-0001

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited

12b. DISTRIBUTION CODE

13. ABSTRACT ***(Maximum 200 Words)***

The most advanced probability density function (PDF) turbulent combustion models were developed and applied to make calculations of turbulent flames. The numerical accuracy of the calculations was carefully studied, and algorithmic improvements were developed. Various turbulence and combustion sub-models were developed and improved. The most significant achievement was the accurate calculation of the Sandia piloted jet nonpremixed flames, including quantitative predictions of local extinction, reignition, and minor species concentrations. Essential ingredients for these successful calculations were: the numerically-accurate particle-mesh method; the augmented reduced chemical mechanism; the in situ adaptive tabulation (ISAT) algorithm; and the Euclidean minimum spanning tree (EMST) mixing model.

14. SUBJECT TERMS
Turbulent Combustion, turbulence modelling, PDF methods

15. NUMBER OF PAGES
15

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	UL